

Off-site-repulsion induced Triplet Superconductivity — a possibility of chiral p_{x+y} pairing in Sr_2RuO_4

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In order to probe the effect of charge fluctuations on triplet pairing, we study the pairing symmetry in the one-band Hubbard model having the off-site Coulomb repulsion (V) on top of the on-site repulsion as a model for the γ band of Sr_2RuO_4 , a strong candidate for triplet pairing superconductor. The result, obtained with the dynamical cluster approximation combined with the quantum Monte-Carlo method, and confirmed from the fluctuation exchange approximation, shows that while $d_{x^2-y^2}$ -pairing dominates over p in the absence of V , introduction of V makes p_{x+y} and d_{xy} dominant. The gap function for the chiral $p_{x+y}+ip_{x-y}$ has nodes that are consistent with the recent measurement of specific heat in rotated magnetic fields in the ruthenate. This suggests that the off-site repulsion may play an essential role in triplet superconductivity in this material.

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Introduction — There has been an increasing fascination with spin-triplet pairing in the condensed matter physics, with a history dating back to the discovery of superfluid ^3He . While triplet superconductivity has been found in some heavy fermion compounds and organic metals, a ruthenate, Sr_2RuO_4 , is prototypical in that its structure is similar to a cuprate La_2CuO_4 , but the replacement of Cu with Ru makes the relevant d orbitals different. So the discovery of superconductivity[1] in the ruthenate has stimulated an enormous amount of studies[2]. Experimentally, it has been established that Sr_2RuO_4 is a chiral (time-reversal broken) triplet superconductor with the spins lying in the RuO_2 plane, where we take the spin quantization axis (z) along the crystalline c -axis, as indicated from Knight shift[3] and μSR [4] experiments.

On the other hand, the symmetry of the gap function, which is of prime importance in identifying the pairing mechanism, has yet to be established. Although the existence of line-nodes in the gap function is suggested from power-law behaviors in specific heat and NMR $1/T_1T$ [2], the position of nodes remains controversial. While the magnetothermal conductivity shows a weak anisotropy in the ab -plane for $T > 0.35\text{K}$ [5, 6], four-fold oscillations [indicative of nodes in the gap function around $\mathbf{k}=(\pm\pi,0)$, $(0,\pm\pi)$] have been detected in a recent measurement of specific heat in rotating magnetic fields by Deguchi *et al.*[7].

One complication is that, unlike the high- T_c cuprates which have a square lattice of $d_{x^2-y^2}$ orbitals, the ruthenate has three, cylindrical Fermi surfaces (labelled as α , β , and γ), where α and β derive from one-dimensional arrays of Ru d_{xz} and d_{yz} orbits, while γ derives from a square lattice of d_{xy} orbits. This has been established experimentally from a de Haas measurement[8] and an angle-resolved photoemission spectroscopy[9] and also confirmed from a first-principles band calculation[10].

Deguchi *et al.* have concluded that their result suggests that the active band for superconductivity is the γ band.[7]

Although various pairing mechanisms have been proposed for Sr_2RuO_4 , they are not straightforward, since it is much more difficult to explain triplet pairing than singlet pairing solely from spin fluctuations because of a smaller pairing interaction in the triplet channel. Several authors[11, 12, 13, 14] have focused on the effect of nesting in the quasi-one-dimensional α - β Fermi surfaces to show that anisotropic antiferromagnetic spin fluctuations, observed in NMR experiment[15], or orbital fluctuations can favor the triplet pairing. On the other hand, assuming that the γ band is the active band for superconductivity, a one-loop renormalization group analysis for the one-band Hubbard model was performed[16], where p -pairing is concluded to be dominant unless the Fermi level is far from the van Hove singularity. A third-order perturbation calculation for the single-band Hubbard model has also been performed *et al.*[17, 18], where triplet pairing is shown to dominate over singlet pairing for intermediate band filling. This was recently extended to the three-band Hubbard model,[18, 19] for which the perturbation calculation shows that triplet pairing remains dominant, residing on the γ band. Their result that the gap function has nodes along [100] for the γ band, while they lie along [110] for α - β , is consistent with the anisotropy in the magnetothermal conductivity[5, 6]. However, we believe that the validity of the results obtained with perturbation expansions, truncated at the third or fourth order, has to be checked by non-perturbative methods.

Indeed, according to the fluctuation exchange (FLEX) study[20] or a phenomenology[21] for the spin fluctuation, triplet pairing is rather weak in general. More specifically, Kuroki *et al.* have shown recently that the singlet pairing dominates over the triplet for the one-

band Hubbard model for the γ band, where they calculated the pairing interaction vertex with the quantum Monte Carlo (QMC) method to show that d -pairing interaction is stronger than those in triplet channels.[22]

Given this background, the motivation of the present study is two-fold. First, we want to clarify whether the triplet superconductivity can be dominant within the one-band Hubbard model in a *non-perturbative* method, for which we have employed the dynamical cluster approximation (DCA) combined with QMC formulated by Jarrell *et al.*[23]. We shall show that $d_{x^2-y^2}$ -wave pairing dominates over p -wave pairings suggested by third-order perturbation studies. Here DCA+QMC is employed for the first time[27] to investigate superconductivity in the extended Hubbard Hamiltonian that models the γ band in the ruthenate.

Second, and more importantly, we propose that the *off-site Coulomb repulsion* can favor triplet superconductivity in general and in the γ band in Sr_2RuO_4 in particular[24]. The underlying physics is that, while we usually evoke spin fluctuations (caused by the on-site repulsion) in considering an electron mechanism of superconductivity, charge fluctuations, which tend to be enhanced by the off-site repulsion, should favor the pairing in the triplet channel, as seen in the expression for the fluctuation-mediated interactions [13, 25]. We have in fact shown with a FLEX calculation that, even for the simple square lattice, transitions between different pairing symmetries can arise due to the coexistence of spin and charge fluctuations[26]. We shall show that the off-site repulsion makes p_{x+y} and d_{xy} dominant while p_x and $d_{x^2-y^2}$ are suppressed. The result is also confirmed by a FLEX calculation. The chiral $p_{x+y} + ip_{x-y}$ gap function then has nodes around $(\pm\pi, 0)$ and $(0, \pm\pi)$, which is consistent with the specific heat in rotating magnetic fields[7].

Formulation — The extended Hubbard model is given as

$$\begin{aligned} \mathcal{H} = & -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) \\ & + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j \rangle, \sigma\sigma'} n_{i\sigma} n_{j\sigma'} \end{aligned}$$

in the standard notation, where nn (nnn) denotes nearest-neighbor (next-nn) sites. In DCA, the original reciprocal space with N points are divided into N_c cells, for which a coarse-graining is done. The Hubbard model is then mapped to a self-consistently embedded cluster of Anderson impurities (rather than a single impurity considered in the dynamical mean-field approximation[28]), so that DCA incorporates nonlocal spatial fluctuations. We have solved the cluster problem generated by the DCA using the QMC with the algorithm proposed by Hirsch and Fye[29]. We choose a cluster size $N_c = 4 \times 4$

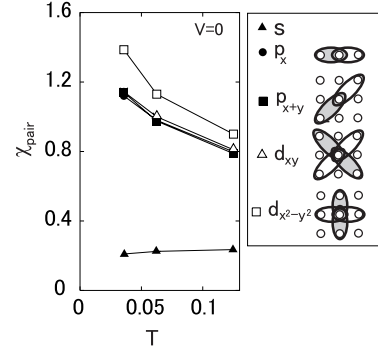


FIG. 1: (a) DCA+QMC result for the pairing susceptibility versus temperature for various symmetries of pairing (depicted in real space in inset) in the on-site Hubbard model ($V = 0$) with the on-site interaction $U = 1.5$, the band filling $n = 1.33$, and $t'/t = 0.4$. Error bars are smaller than the size of each symbol.

throughout the study[30].

The effect of the off-site repulsion V can be incorporated into the DCA calculation as follows. The off-site term is expressed in k -space as

$$\sum_{\langle i,j \rangle, \sigma\sigma'}^{nn} V_{ij} n_{i\sigma} n_{j\sigma'} = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} V\mathbf{q} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}'\sigma}^\dagger c_{\mathbf{k}'-\mathbf{q}\sigma}$$

with $V\mathbf{q} = (V/N)[\cos(q_x) + \cos(q_y)]$, which has to be coarse-grained. One might think that the coarse-graining may introduce interactions extending beyond nearest neighbors for the impurity cluster model. However, we can note a relation, $\tilde{V}\mathbf{Q} \equiv (N_c/N) \sum_{\tilde{\mathbf{q}}} V\mathbf{Q} + \tilde{\mathbf{q}} = (\tilde{V}/N_c)(\cos Q_x + \cos Q_y)$, where the summation for $\tilde{\mathbf{q}}$ runs over the momenta in the coarse-graining cell centered at \mathbf{Q} , and $\tilde{V} \equiv \sin(\pi/N_c)/(\pi/N_c)V$. Thus the form of the interaction does not change, so we have only to consider the off-site repulsion \tilde{V} in the QMC for the impurity cluster model.

Results — In the DCA+QMC calculation, we take the half of the band width as the unit of energy as customary done. We take the on-site Coulomb interaction $U = 1.5$, the band filling $n = 1.33$, and $t'/t = 0.4$. These values are chosen to roughly represent the γ band of the ruthenate. The pairing symmetries considered are $s \sim 1$, $p_x \sim \sqrt{2} \sin(k_x)$, $p_{x\pm y} \sim \sqrt{2} \sin(k_x \pm k_y)$, $d_{x^2-y^2} \sim \cos(k_x) - \cos(k_y)$, and $d_{xy} \sim \cos(k_x + k_y) - \cos(k_x - k_y)$, as depicted in real space in the inset of Fig.1. We first show the result before V is turned on. Figure 1 shows the pairing susceptibility for the on-site Hubbard model as a function of temperature, where $L = 64$ Trotter-Suzuki decomposition number is taken. We can see that $d_{x^2-y^2}$ is the dominant pairing, while p_{x+y} is weaker in the region $T \geq 0.031$ studied here. The result is consistent with Ref.[22], where $d_{x^2-y^2}$ is shown to dominate over triplet pairings by a QMC for a finite ($N = 14 \times 14$) Hubbard

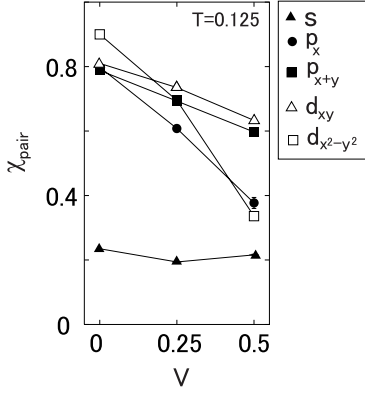


FIG. 2: The pairing susceptibility in the extended Hubbard model as a function of the off-site repulsion V for $U = 1.5$, $n = 1.33$, and $t'/t = 0.4$ at $T = 0.125$. Error bars are smaller than the size of each symbol.

model with $U = 0.5$. These results, obtained with non-perturbative methods, suggest that the on-site Hubbard model is insufficient to describe the superconductivity in Sr_2RuO_4 .

Now we move on to the extended Hubbard model in Fig.2, where the DCA+QMC result for the pairing susceptibility is plotted as a function of the off-site interaction V for $T = 0.125$ with the Trotter-Suzuki decomposition number $L = 24$. We can clearly see a qualitative tendency that p_{x+y} and d_{xy} become dominant with the introduction of V , while p_x and $d_{x^2-y^2}$ are suppressed. Physically, this should be because the nearest-neighbor V suppresses pairs formed across nearest-neighbor sites, while the pairs such as p_{x+y} and d_{xy} that are formed across more distance sites (see the inset of Fig.1) are less affected. We cannot take a lower T or larger L at present, since in the QMC algorithm for $V \sum n_{i\sigma} n_{i\sigma'}$ eight Hubbard-Stratonovich auxiliary fields (for $\sigma, \sigma' = \uparrow, \downarrow$ for x, y directions) are needed on top of the one for the U -term, so the study of the subtle competition between p_{x+y} and d_{xy} at lower temperatures is a future study[32].

Still, it is interesting to discuss what should result from the p -wave pairing. Below T_c the p_{x+y} -wave pairing is expected to take a chiral form,

$$p_{x+y} + ip_{x-y} \sim \sin(k_x + k_y) + i \sin(k_x - k_y),$$

since the mixing should increase the gap energy ($|\Delta|$). We can then note, as depicted in Fig.3, that the gap function Δ for the $p_{x+y} + ip_{x-y}$ has nodes (or minima of $|\Delta|$) on the Fermi surface at around $(\pm\pi, 0)$ and $(0, \pm\pi)$ (which happen to be similar to those for the chiral $p_x + ip_y \sim \sin(k_x) + i \sin(k_y)$; Fig.3(b)). So the chiral $p_{x+y} + ip_{x-y}$ is consistent with the specific heat measurement[7], and should be a candidate for the triplet superconductivity in Sr_2RuO_4 .

We finally examine whether the FLEX, a renormal-

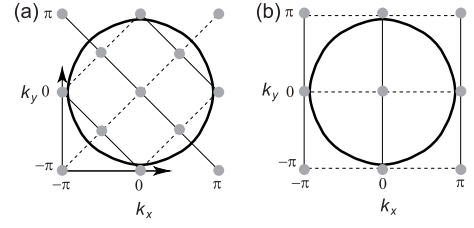


FIG. 3: (a) The position of nodes of $p_{x+y} \sim \sin(k_x + k_y)$ (solid lines), $p_{x-y} \sim \sin(k_x - k_y)$ (dotted), and $p_{x+y} + ip_{x-y}$ (gray dots). The bold solid curve represents the γ Fermi surface of Sr_2RuO_4 . (b) A plot similar to (a) for $p_x + ip_y \sim \sin(k_x) + i \sin(k_y)$.

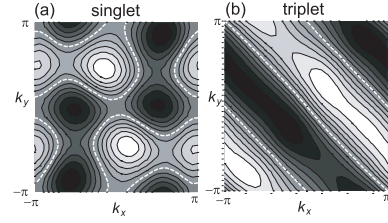


FIG. 4: Contour plot of the gap function for the singlet(a) and triplet(b) pairs obtained with FLEX+Eliashberg's equation for the extended Hubbard model for $U = 2.5$, $V = 0.65$, $n = 1.33$, $t'/t = 0.5$, and $T = 5 \times 10^{-3}$. White dashed lines denote the nodes. For (b), another one, rotated by 90 degrees, is degenerate.

ized perturbation, would reproduce the above result. The FLEX was first formulated by Bickers *et al.*[33] for the Hubbard model, and further applied to the extended Hubbard model by Esirgen *et al.*[34]. We first obtain the renormalized Green's function, G , taking bubble and ladder diagrams as the self energy. We then calculate the pairing interaction mediated by spin and charge fluctuations, and plug that in Eliashberg's equation,

$$\lambda\phi(k) = -\frac{T}{N} \sum_{k'} \Gamma^{\text{PP}}(k - k') G(k') G(-k') \phi(k'), \quad (1)$$

where ϕ is the gap function, $k \equiv (\mathbf{k}, \omega_n)$ with ω_n being Matsubara frequency, and Γ^{PP} the pairing interaction between the pairs with $(\mathbf{k}, -\mathbf{k})$ and $(\mathbf{k}', -\mathbf{k}')$.

The maximum eigenvalue λ becomes unity when T becomes the transition temperature of the dominant pairing. We take $N = 32 \times 32$ sites at temperature $T = 5 \times 10^{-3}$ and $-(2N_c - 1)\pi T \leq \omega_n \leq (2N_c - 1)\pi T$ with $N_c = 1024$. When the off-site interaction V is introduced all the vertices and susceptibilities become $(Z + 1) \times (Z + 1)$ matrices for the lattice coordination number $Z (= 4$ for the square lattice).

We have performed the FLEX calculation for $t'/t = 0.4, 0.5$, $n = 1.33$, $U = 1.5 - 2.5$, $V = 0 - U/4$. While the singlet pairing is dominant in most of the parameter

region, we have found that the maximum eigenvalue of Eliashberg's equation becomes greater for triplet pairing than that of the singlet for $0.625 \leq V \leq 0.675$ for $U = 2.5$ [35]. Figure 4 depicts the gap functions for triplet and singlet cases. The symmetry of the gap function, which is p_{x+y} - and d_{xy} -like, respectively, does agree with the above DCA+QMC result.[36]

In summary, we have found using DCA+QMC and FLEX methods that, while p -wave pairing is weaker than $d_{x^2-y^2}$ in the on-site Hubbard model, introduction of the off-site repulsion V suppresses p_x and $d_{x^2-y^2}$, making p_{x+y} and d_{xy} more favorable. Although the effect of α and β bands is beyond the scope of the present study, the qualitative tendency of the present work that the off-site repulsion acts to preferentially suppress nearest neighbor pairs should hold for multibands as well as for single bands. The position of the nodes in the gap function for the chiral $p = p_{x+y} + ip_{x-y}$ is consistent with a specific heat measurement for Sr_2RuO_4 [7], so this is a promising candidate for the triplet superconductivity in Sr_2RuO_4 , and the off-site repulsion may play an essential role there.

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gap function due to a mixing with $d_{x^2-y^2}$.